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This Augmentation Award for Science and Engineering Research Training (AASERT) supported research students to work on adaptive and parallel computational techniques associated with crystal growth processing. This grant accompanied the AFOSR Multidisciplinary Univer-sity Research Initiative (MURI) in crystal growth which is centered at the State University of New York at Stony Brook. Students conducted research on the following topics.

Systems integration tools to enable the various software components to interact and, thus, address the simulation of the entire crystal-growth manufacturing process.

Software for parallel adaptive computation that may be used by the crystal growth con-sortium to solve finite element and finite volume problems. The tools will be capable of solving transient and steady problems on serial and parallel computers using adaptive h-, p-, and r-refinement.

Unstructured-grid flow analysis software that may bc used to address problems in complex geometrical configuratioxm, e.g., in the vicinity of the radiative heater of a Czochralski process.

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(AASERT95) ADAPTIVE AND PARALLEL COMPUTATIONAL TECHNIQUES IN MATERIALS SCIENCE

Final Report

1 June 1995 - 31 May, 1998

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1 Introduction

This Augmentation Award for Science and Engineering Research Training (AASERT) supported research students to work on adaptive and parallel computational techniques associated with crystal growth processing. This grant accompanied the AFOSR Multidisciplinary University Research Initiative (MURI) in crystal growth which is centered at the State University of New York at Stony Brook. Students conducted research on the following topics.

- Systems integration tools to enable the various software components to interact and, thus, address the simulation of the entire crystal-growth manufacturing process.
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- Unstructured-grid flow analysis software that may be used to address problems in complex geometrical configurations, e.g., in the vicinity of the radiative heater of a Czochralski process.

A more detailed description of this work follows.

2 Research Accomplishments

2.1 Global Systems Integration

We developed integrated software components involving:

1. radiative heat transfer analysis based on Naraghi's discrete exchange factor method to account for the thermal exchange between the radiative heaters and the outer crucible walls;

2. unsteady heat-conduction analysis based on a three-dimensional, hierarchical, adaptive hp-refinement, finite element method to compute heat transfer through the crucible walls to the melt flow; and

3. unsteady melt-flow analysis based on the multizone adaptive scheme for transport and phase-change processes (MASTRAPP) to determine the fluid flow and crystal formation.

The three component software systems were developed, respectively, at Manhattan College, Rensselaer, and Stony Brook, so interfaces had to be created for an integrated thermal analysis of a crystal-growth configuration. The radiative-analysis software is currently axisymmetric while the heat-conduction software is three dimensional. Temperatures from the heat-conduction software are projected onto the lower-dimensional space for radiative analysis and the dimensionality of the radiative results are expanded. Since each software system uses different unstructured data structures, care was needed to ensure efficiency. This was made possible by the hierarchical structures within the adaptive system used for the heat-conduction analysis. A Schwarz alternation strategy was established between the radiative and conduction processes where the radiative software provides fluxes to the conduction software and the conduction software provides temperatures to the radiation software.

The interface between the heat-conduction and two-dimensional Mastrapp software operates in similar fashion with temperatures on the inner crucible surface obtained from the MASTRAPP flow analysis and the heat-conduction software providing fluxes to MASTRAPP. The solution process proceeds iteratively in a relatively efficient manner.

An example involving a crucible containing indium phosphide (InP) was solved to evaluate the software. The processing system contains two radiative heaters: one surrounding the lateral surfaces and the other at the bottom of the crucible. In Figure 2.1, we show the flow patterns and temperature contours on the crucible walls produced by the combined radiation, heat conduction, and flow analysis.

The process of making three, large, independent software systems operate in harmony was a major step forward. With this system in place, accurate appraisals of the influence of heater placement and thermal variations on the flow and resulting crystal may be evaluated and understood. With direct access to the heater control, it is now possible to investigate strategies for process control. These results were reported in Hongwei Li's Computer Science MS project.

2.2 Finite Element Flow Analysis

We have been using K. Jansen's ENSA system to solve melt flow problems. ENSA uses a stabilized finite element solution strategy and contains capabilities for large eddy simulation (LES) of three-dimensional turbulent flows. The ENSA software will be used to analyze melt flows and gaseous flows surrounding the crystal and in the vicinity of the radiative heater. In order to improve performance of the flow software, we have developed procedures for generating boundary-layer meshes which are only graded in a direction normal to the layer. These meshes will greatly improve the efficiency of the solution procedures at high Grashof numbers.

2.3 Parallel Computation

The flow software can operate in either a serial or parallel computational mode. Parallel computational capabilities include distribution of the mesh and solution data across the processors of the computer, dynamic load balancing by a variety of techniques, partition boundary traversal and information updating, and mesh migration.

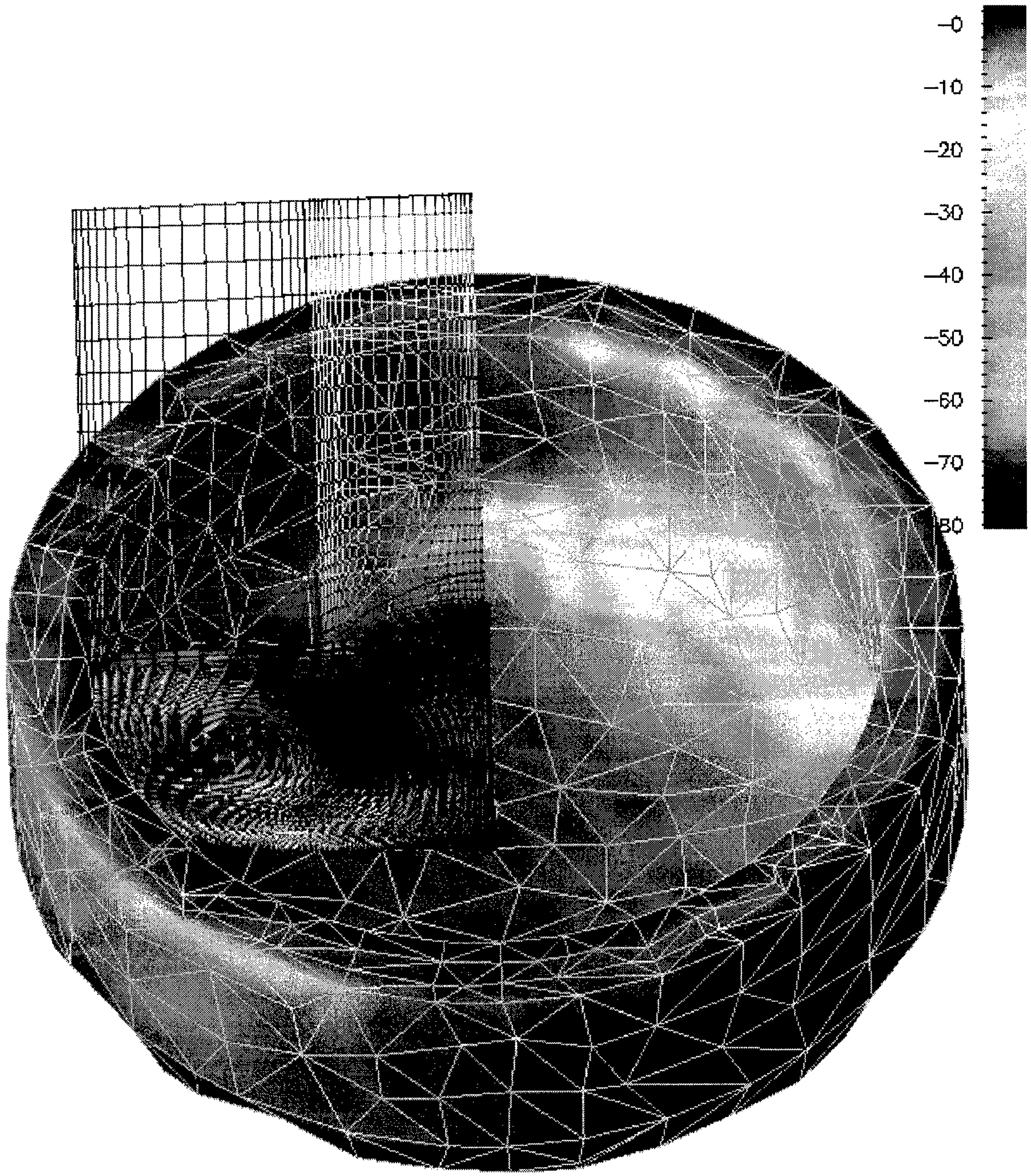

Figure 1: Systems analysis of the radiative heat transfer to a crucible containing InP.

The application should not change when operating in parallel. To achieve this, we create a hierarchical *partition model*, analogous to the geometric model used to classify geometric entities onto a domain. All entities classified on a single partition model entity are assigned to a specific processor, but multiple partition model entities may be assigned to a single process. Partition model entities are classified on a *process model* and process model entities are classified on a *machine model*. The machine model represents the physical processors, and information about the communication methods to other computers in the processing. The process model maps the process to the computer, and maps interprocessor communication to inter-computer networks or, perhaps, to a shared-memory interface.

Our target architectures include computers with SMP nodes connected by a network. Each thread of execution in a parallel computation is assigned a process model entity, which is in turn classified on the machine model. A machine model entity represents a processing node, which may have multiple processing units. Multiple partitions can be assigned to a single process. Multiple processes can be assigned to a single computer, in cases where a machine has multiple processors (SMP) or when running multiple processes on a single CPU. The machine model can be used to model different network speeds. Mesh migration is achieved by reclassifying part of the mesh on a new partition model entity, then moving that partition model entity to a new processor (reclassifying it on the processor model). Boundaries between submeshes which are classified on different partition models but which live on the same processor do not require duplicated entities and can access information from the neighboring process without communication. This model will allow us to take advantage of such information during partitioning and load balancing.

3 Publications

1. D. Givoli, J.E. Flaherty and M.S. Shephard, "Parallel Adaptive 3D Finite Element Analysis of CZ Melt Flows," *J. Crystal Growth*, **174** (1997), 1-6.

2. D. Givoli, J.E. Flaherty and M.S. Shephard, "Parallel Adaptive Finite Element Analysis of Viscous Flows with Application to Czochralski Melt Flows," *Int. J. Num. Meth. Heat Fluid Flow*, **7** (1997), 880 - 906. Awarded best paper of the year 1997 in the journal by the Literati Society.

3. D. Givoli, J.E. Flaherty and M.S. Shephard, "3D "Analysis of InP LEC Melt Flows Using a Parallel Adaptive Finite Element Scheme," *J. Crystal Growth*, **180** (1997), 510-516.

4. S. Adjerid, A. Aiffa, J.E. Flaherty, J.B. Hudson, and M.S. Shephard, "Modeling and Adaptive Numerical Techniques for Oxidation of Ceramic Composites," *Ceramic Engng. and Sci. Procs.*, **18** (1997), 315-322.

5. Q. Yan, "Computational Methods for Radiation Problems," M.S. Project, Dept. Comp. Sci., Rensselaer Polytechnic Institute, Troy, 1997.

6. R. Garimella, M.S. Shephard, and B.E. Webster, "Automatic Mesh Generation of Complex Configurations Including Viscous Boundary Layers," Proc. 10th Int. Conf. on Finite Elements in Fluids, 1998, to appear.

7. J.E. Flaherty, R.M. Loy, C. Ozturan, M.S. Shephard, B.K. Szymanski, J.D. Teresco, and L.H. Ziantz, "Parallel Structures and Dynamic Load Balancing for Adaptive Finite Element Computation," *Appl. Numer. Maths.*, **26** (1998), 241-265.

8. S. Adjerid, J.E. Flaherty, K. Jansen, and M.S. Shephard, "Parallel Finite Element Simulations of Czochralski Melt Flows," *Proc ICES '98*, submitted, 1998.

9. Hongwei Li, *Interdisciplinary Thermal Analysis in the Czochralski Crystal Growth Process Using a hp Adaptive Finite Element Environment*, M.S. Project, Dept. Comp. Sci., Rensselaer Polytechnic Institute, Troy, 1998.

10. J.D. Teresco, M.W. Beall, J.E. Flaherty, and M.S. Shephard, "A Hierarchical Partition Model for Adaptive Finite Element Computation," *Comp. Meths. Appl. Mech. Engng.*, submitted, 1998.

4 Supported Students

1. Ph.D. Student James Teresco, July 1, 1995 - May 31, 1998

2. Ph.D. Student Wesley Turner, July 1, 1995 - August 31, 1997